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Comparison of the local structural stabilities of mammalian prion protein (PrP) by fragment molecular orbital calculations

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	Secondary Structure Elements	Internal Interaction Energies ΔE^{Int} / kcal mol^{-1}							
		Human	Bovine	Mouse	Hamster	Dog	Cat	Average[a]	σ [b]
					Neutral pH models				
1	β1	–30	–33	–42	–30	–23	–39	–33	7
2	L1	–154	–188	–149	–84	–180	–79	–139	47
3	α1	–568	–568	–555	–609	–552	–635	–581	34
4	L2	–41	–34	–39	–52	–42	–41	–42	6
5	β2	–37	–39	–43	–36	–21	–53	–38	10
6	L3	–162	–180	–150	–207	–102	–152	–159	35
7	α2	–648	–731	–668	–666	–613	–562	–648	57
8	L4	–58	–62	–47	–40	–51	–61	–53	9
9	α3	–724	–796	–787	–851	–749	–713	–770	52
	Total[c]	–2422	–2631	–2480	–2575	–2333	–2335		
					Mildly acidic pH models				
1	β1	–29	–30	–42	–32	–23	–38	–32	7
2	L1	–123	–162	–118	–61	–143	–62	–112	42
3	α1	–617	–607	–554	–605	–551	–629	–594	33
4	L2	–44	–38	–44	–57	–43	–42	–44	6
5	β2	–40	–39	–44	–36	–22	–53	–39	10
6	L3	–166	–174	–150	–207	–108	–150	–159	33
7	α2	–620	–746	–607	–648	–566	–522	–618	77
8	L4	–61	–57	–45	–43	–48	–65	–53	9
9	α3	–729	–798	–791	–860	–764	–714	–776	53
	Total[c]	–2429	–2651	–2395	–2549	–2268	–2275		

Table S1. The internal interaction energies (ΔE^{Int}) for the secondary structure elements on PrP models under neutral and mildly acidic pH conditions. [a]The average for the values of ΔE^{Int}. [b]The standard deviations σ for the values of the ΔE^{Int}. [c]Sum over the values of ΔE^{Int}.

	Secondary Structure Element Pairs			Pair Interaction Energies, ΔE^{Pair} /kcal mol^{-1}							
				Human	Cattle	Mouse	Hamster	Dog	Cat	Average [a]	σ[b]
1	β1	–	L1	–29	–32	–34	–16	–23	–20	–26	7
2	β1	–	α1	+0	+0	+0	+0	–0	+0	+0	0
3	β1	–	L2	–1	+0	–2	–0	–0	–0	–0	1
4	β1	–	β2	–27	–22	–24	–17	–25	–36	–25	6
5	β1	–	L3	–28	–31	–17	–25	–28	–13	–24	7
6	β1	–	α2	–3	–3	–22	–1	–10	–5	–7	8
7	β1	–	L4	+0	–0	+0	+0	+0	+0	+0	0
8	β1	–	α3	–1	+2	–7	+2	–4	–3	–2	4
9	L1	–	α1	–141	–85	–196	–182	–129	–104	–139	43*
10	L1	–	L2	–56	–76	–34	–24	–100	–36	–54	29*
11	L1	–	β2	–10	–14	–14	–10	–14	–9	–12	2
12	L1	–	L3	–18	+3	+6	+5	+5	+4	+1	9
13	L1	–	α2	+111	+88	+95	+110	+98	+110	+102	10
14	L1	–	L4	–32	–39	–30	–37	–28	–31	–33	4
15	L1	–	α3	–130	–92	–67	–65	–134	–93	–97	30*
16	α1	–	L2	–20	–33	–26	–23	–5	–28	–22	9
17	α1	–	β2	+0	–0	+0	+0	+0	+0	+0	0
18	α1	–	L3	+1	+1	–3	–2	–2	–1	–1	1
19	α1	–	α2	+10	+6	–50	–59	–46	–30	–28	30*
20	α1	–	L4	–48	–93	–4	–3	+9	+5	–22	40*
21	α1	–	α3	–48	–40	–80	–22	+10	–48	–38	30*
22	L2	–	β2	–19	–26	–22	–23	–17	–13	–20	4
23	L2	–	L3	–0	+1	+1	+1	–3	+1	–0	2
24	L2	–	α2	–20	–15	–13	–33	–58	–13	–25	18
25	L2	–	L4	–1	–1	+0	–1	+19	+1	+3	8
26	L2	–	α3	–13	–14	–9	–8	+35	–8	–3	19
27	β2	–	L3	–15	–6	–13	–22	–13	–13	–14	5
28	β2	–	α2	–35	–16	–18	–27	–24	–1	–20	11
29	β2	–	L4	+1	+1	+1	+1	+1	+1	+1	0
30	β2	–	α3	–21	–23	–40	–27	–18	–12	–23	10
31	L3	–	α2	–68	–24	–23	–44	–26	–54	–40	19
32	L3	–	L4	+7	–2	–3	–3	–3	–2	–1	4
33	L3	–	α3	+41	–13	–20	–39	–12	–10	–9	27*
34	α2	–	L4	–115	–95	–111	–171	–128	–115	–122	26*
35	α2	–	α3	–237	–143	–167	–225	–216	–274	–211	48*
36	L4	–	α3	–3	–6	–9	+2	+10	+28	+4	14
	Total			–966	–843	–954	–988	–880	–822		

Table S2. The pair interaction energies (ΔE^{Pair}) of 6 PrPs under mildly acidic pH condition. The pair interaction energies were evaluated by summing over the calculated IFIEs between the residues on the elements pairs. [a] The average of ΔE^{Pair}. [b] The standard deviations of ΔE^{Pair}. [c] *: $\sigma \geq 20$ kcal/mol. The blue-marked ΔE^{Pair} boxes are the maximum value (most repulsive interaction) among the species. The red-marked ΔE^{Pair} boxes are the minimum value (most attractive interaction) among the species.

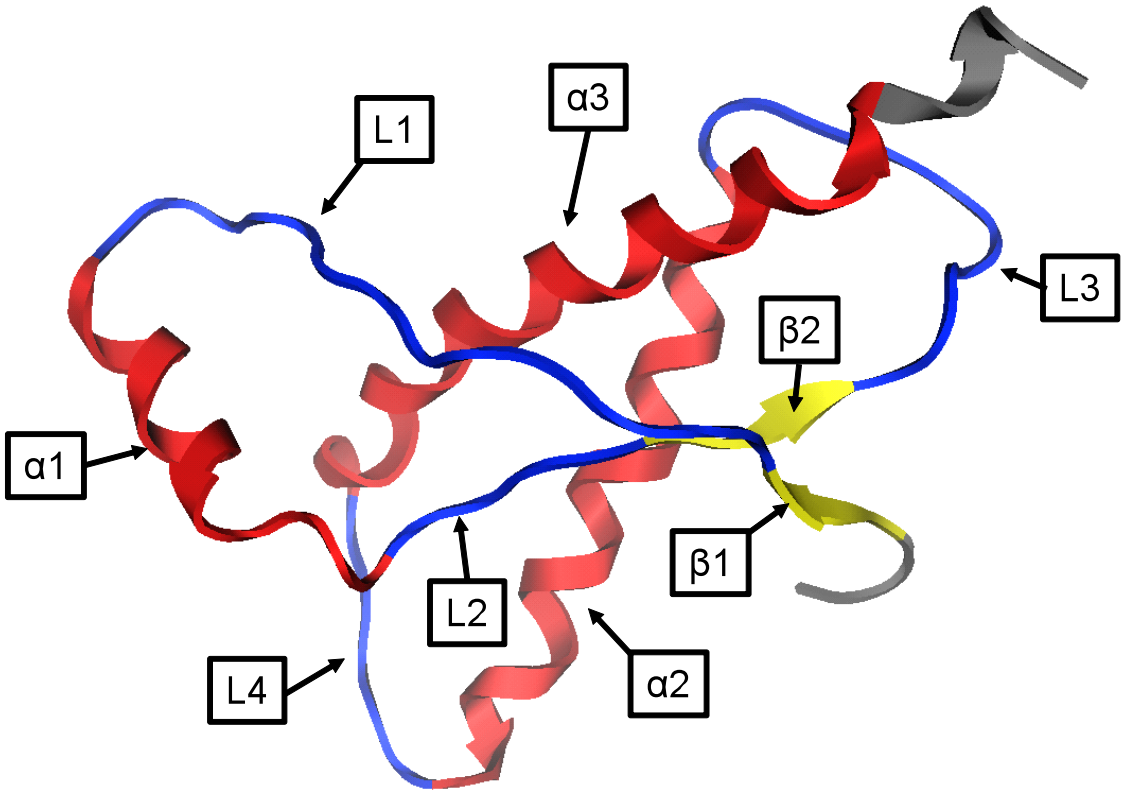

Fig. S1. The secondary structure elements of PrP: three α-helices (α1, α2 and α3); two β-strand (β1 and β1); four loops (L1, L2, L3 and L4).

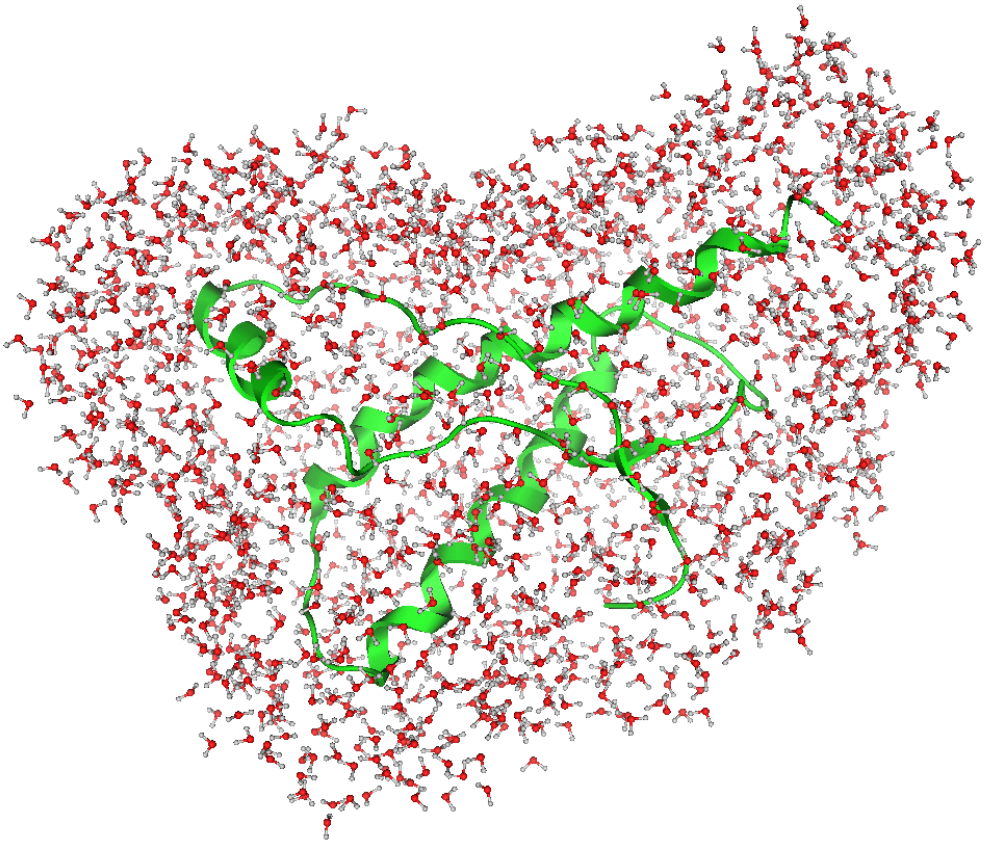

Fig. S2. Example of PrP structural models in water that used in FMO calculations. Human PrP protein of the first conformer deposited in PDB (code 1QM3) rendered as green-colored ribbon type was immersed by 1643 water molecules depicted as ball-and-stick type.